Journal of Computational and Applied Mathematics 224 (2009) 415–432

Contents lists available at ScienceDirect

Journal of Computational and Applied Mathematics

journal homepage: www.elsevier.com/locate/cam

Scheifele two-step methods for perturbed oscillators

Hans Van de Vyver

Royal Meteorological Institute of Belgium, Avenue Circulaire 3, B-1180 Brussels, Belgium

ARTICLE INFO

Article history:
Received 2 February 2008
Received in revised form 27 April 2008

MSC:
65L05

Keywords:
Two-step methods
Perturbed oscillators
Scheifele's *G*-function method
Linear stability
Phase-lag
Satellite problem

ABSTRACT

Two-step methods specially adapted to the numerical integration of perturbed oscillators are obtained. The formulation of the methods is based on a refinement of classical Taylor expansions due to Scheifele [G. Scheifele, On the numerical integration of perturbed linear oscillating systems, Z. Angew. Math. Phys. 22 (1971) 186–210]. The key property is that those algorithms are able to integrate exactly harmonic oscillators with frequency ω. The methods depend on a parameter $\nu = \omega h$, where h is the stepsize. Based on the B2-series theory of Coleman [J.P. Coleman, Order conditions for a class of two-step methods for $y'' = f(x, y)$, IMA J. Numer. Anal. 23 (2003) 197–220] we derive the order conditions of this new type of method. The linear stability and phase properties are examined. The theory is illustrated with some fourth- and fifth-order explicit schemes. Numerical results carried out on an assortment of test problems (such as the integration of the orbital motion of earth satellites) show the relevance of the theory.

1. Introduction

In the last decade, there has been a great interest in the research of methods for the numerical integration of initial value problems (IVP) associated to second-order ordinary differential equations (ODE)

$$y'' = f(x, y), \qquad y(x_0) = y_0, \qquad y'(x_0) = y'_0, \tag{1.1}$$

in which the first derivative does not appear explicitly. These problems appear often in practice. Of course, since (1.1) can be written as an IVP for a system of two equations of first order, the problem can be solved by algorithms for first-order equations. However, this will be less efficient if methods specially devised for the given problem would be used. The construction of methods specialized for (1.1) is a well established area of investigation. Many multistep methods (such as Störmer–Cowell methods) and two-step methods for (1.1) have been developed, see for example [19,1–4,24–26,28,13] to mention a few. Two-step methods are considered to be more efficient than Runge–Kutta–Nyström methods for (1.1). For example, the standard fourth-order explicit Runge–Kutta–Nyström method (see [16]) requires three function evaluations whereas the fourth-order explicit Numerov method of [1] requires only two function evaluations per step.

Quite often the solution of (1.1) exhibits an oscillatory behaviour; think, for instance, of the pendulum problem in celestial mechanics or of the Schrödinger equation in quantum mechanics. For problems having highly oscillatory solutions standard methods with unspecialized use can require a huge number of steps to track the oscillations. One way to obtain a more efficient integration process is to construct numerical methods with an increased order. On the other hand, the construction and implementation of high-order methods is not evident. Alternatively, one can consider methods that use the detailed information of the high-frequency oscillation. There is a vast literature on this subject; an extensive bibliography is summarized in [22]. Scheifele [23] was concerned with the solution of *perturbed oscillators*, i.e., second-order problems of the form

$$y'' = -\omega^2 y + g(x, y), \qquad y(x_0) = y_0, \qquad y'(x_0) = y'_0, \tag{1.2}$$

E-mail address: hans_vandevyver@hotmail.com.

0377-0427/$ – see front matter © 2008 Elsevier B.V. All rights reserved.
doi:10.1016/j.cam.2008.05.010

where the magnitude of the perturbation force satisfies $|g(x,y)| \ll \omega^2\,|y|$. Scheifele rewrote the solution of (1.2) as a series of a set of functions, the G-functions, more adequate to perturbed oscillators than the classical polynomial Taylor expansion. The Scheifele G-function method is capable of integrating exactly the harmonic oscillator or unperturbed problem (i.e. (1.2) with $g = 0$). In spite of its excellent behaviour, the Scheifele G-function method has the disadvantage that it is strictly application dependent. Several authors have applied Scheifele's approach for constructing numerical methods adapted to perturbed oscillators. Most of these papers are focused on space dynamical problems such as an accurate integration of orbit problems or long-term prediction of satellite orbits. Some Scheifele G-functions based multistep codes are designed in [21]. Also adapted methods without first derivatives have been constructed in [20]. A first Runge–Kutta type version of the Scheifele G-function method is due to González et al. [15]. A theoretical foundation for these adapted Runge–Kutta–Nyström (ARKN) methods is given in [10–12,14].

Our objective in this paper is to apply Scheifele's approach to two-step methods. This was already proposed in [30] for the simple explicit Numerov method. The excellent numerical results reported in that paper strongly suggest constructing higher-order methods of this type. This is possible when a more theoretical framework would be developed. This is the purpose of this work. The paper is organized as follows. Section 2 is of an introductory nature: we recall a class of classical two-step (TS) methods. In Section 3 we recall Scheifele's approach. This idea will be extended to TS methods, the resulting methods are denoted by STS methods. Section 4 is devoted to the order conditions for STS methods. This part heavily relies on the work in [4] for classical TS methods. Some general stability results for STS methods are reported in Section 5. The concepts of such a stability analysis find its origin in the work in [5,12]. Section 6 provides general results on the phase properties of STS methods. The analysis is based on the work in [12]. Section 7 deals with the construction of fourth- and fifth-order explicit STS methods. Several possibilities are explored such as minimizing the error constant, increasing the phase-lag order, dissipative or not, etc. The classical companions of the new methods are previously derived in [13]. Section 8 collects numerical examples for a variety of problems chosen to illustrate particular features of the STS methods obtained. The new methods are compared with other high-quality methods. The paper concludes with a brief summary of the work considered here.

2. Classical two-step methods

Two-step (TS) methods for (1.1) are defined by

$$Y_i = (1+c_i)\,y_n - c_i\,y_{n-1} + h^2 \sum_{j=1}^{s} a_{ij}\,f(x_n + c_j\,h, Y_j), \quad i = 1,\dots,s, \tag{2.3}$$

$$y_{n+1} = 2\,y_n - y_{n-1} + h^2 \sum_{i=1}^{s} b_i\,f(x_n + c_i\,h, Y_i), \tag{2.4}$$

where y_{n-1}, y_n and y_{n+1} are approximations of $y(x_n - h)$, $y(x_n)$ and $y(x_n + h)$, respectively. TS methods can be represented in short-hand notation by the Butcher table

$$\begin{array}{c|ccc} c_1 & a_{11} & \dots & a_{1s} \\ \vdots & \vdots & \ddots & \vdots \\ c_s & a_{s1} & \dots & a_{ss} \\ \hline & b_1 & \dots & b_s \end{array} = \begin{array}{c|c} c & A \\ \hline & b^{\mathrm{T}} \end{array},$$

where $c, b \in \mathbb{R}^{s\times 1}$ and $A \in \mathbb{R}^{s\times s}$. These coefficients are derived by imposing the necessary and sufficient conditions for *convergence*, i.e. *consistency* and *zero-stability*, see [17] for the general theory.

For exact starting values, the *local truncation error (lte)* of the method at x_n is

$$lte = y(x_n + h) - y_{n+1}.$$

The method is of *order* p if $lte = \mathcal{O}(h^{p+2})$. The *principal local truncation error (plte)* is the leading term of the *lte*. For a pth-order method this is of the form

$$plte = \frac{h^{p+2}}{(p+2)!} \sum_{\substack{t\in T_2 \\ \rho(t)=p+2}} \alpha(t)\,\left(1 + (-1)^{p+2} - b^{\mathrm{T}}\,\Psi''(t)\right) F(t)(y_n, y_n'), \tag{2.5}$$

where $\alpha(t)$, $\rho(t)$, $\Psi''(t)$, $F(t)$ and T_2 are defined in [4]. The coefficients of $F(t)(y_n, y_n')$ in (2.5) will be denoted as $e_{p+1}(t)$. The quantity

$$E_{p+1} = \left(\sum_{\substack{t\in T_2 \\ \rho(t)=p+2}} e_{p+1}^2(t) \right)^{1/2}, \tag{2.6}$$

will be called the *error constant* of the pth-order method. Traditionally, the order conditions for TS methods are usually derived by expansions in Taylor series. These expansions are calculated essentially by brute force. On the other hand, Coleman [4] obtained the order conditions for TS methods by using the theory of B-series. Analogously to the case of RK(N) methods, the determination of the order of a TS method is based on checking certain relationships between the coefficients of the method.

The linear stability analysis of methods for solving (1.1) is based on the scalar test equation (see [19])

$$y'' = -\lambda^2 y. \tag{2.7}$$

An application of a TS method to (2.7) yields

$$\begin{aligned} Y &= (e+c)\, y_n - c\, y_{n-1} - H^2 A\, Y, \quad H = \lambda\, h, \\ y_{n+1} &= 2\, y_n - y_{n-1} - H^2\, b^{\mathrm{T}}\, Y, \end{aligned} \tag{2.8}$$

where $Y = (Y_1, \ldots, Y_s)^{\mathrm{T}}$ and $e = (1, \ldots, 1)^{\mathrm{T}} \in \mathbb{R}^{s\times 1}$. Elimination of the vector Y from (2.8) results in the difference equation

$$y_{n+1} - S(H^2)\, y_n + P(H^2)\, y_{n-1} = 0, \tag{2.9}$$

where

$$\begin{aligned} S(H^2) &= 2 - H^2\, b^{\mathrm{T}}\, (I + H^2 A)^{-1}\, (e+c), \\ P(H^2) &= 1 - H^2\, b^{\mathrm{T}}\, (I + H^2 A)^{-1}\, c. \end{aligned} \tag{2.10}$$

The solution of the difference equation (2.9) is determined by the *characteristic equation*

$$\xi^2 - S(H^2)\, \xi + P(H^2) = 0. \tag{2.11}$$

Of particular interest for periodic motion is the situation where the roots of (2.11) lie on the unit circle. For example, in celestial mechanics it is desired that numerical orbits do not spiral inwards or outwards. This periodicity condition is equivalent to

$$P(H^2) = 1 \quad \text{and} \quad |S(H^2)| < 2, \quad \forall H \in (0, H^2_{\mathrm{per}}), \tag{2.12}$$

and the interval $(0, H^2_{\mathrm{per}})$ is called the *interval of periodicity*. The method is said to be *periodic (P)-stable* when the interval of periodicity is $(0, \infty)$. If the necessary condition $P(H^2) = 1$ to have a non-empty interval of periodicity is not satisfied, we can ask when the numerical solution remains bounded. This stability condition is equivalent to

$$P(H^2) < 1 \quad \text{and} \quad |S(H^2)| < 1 + P(H^2), \quad \forall H \in (0, H^2_{\mathrm{stab}}),$$

and the interval $(0, H^2_{\mathrm{stab}})$ is called the *interval of absolute stability*.

Another related concept, which is important when solving problems of the form (1.1) is the phase-lag of the method. In phase analysis one compares the phases of $\exp(\pm \mathrm{i}\, H)$ with the phases of the roots of the characteristic equation (2.11). Following the approach in [32] for RKN methods, the quantities

$$\phi(H) = H - \arccos\left(\frac{S(H^2)}{2\sqrt{P(H^2)}}\right), \qquad d(H) = 1 - \sqrt{P(H^2)}, \tag{2.13}$$

are the *phase-lag (or dispersion)* and the *dissipation (or amplification error)*, respectively. The method is said to have *phase-lag order* q and *dissipation order* r if

$$\phi(H) = c_\phi\, H^{q+1} + \mathcal{O}(H^{q+3}), \qquad d(H) = c_d\, H^{r+1} + \mathcal{O}(H^{r+3}).$$

The constants c_ϕ and c_d are called the *phase-lag* and *dissipation constants*, respectively. Methods with $d(H) = 0$ are *zero-dissipative*. Likewise, when $d(H) \neq 0$ the method is *dissipative*.

3. Two-step methods for perturbed oscillators

3.1. Notations and exact solution

Although, Scheifele's method is based on G-functions, in this paper we consider the related ϕ-functions which are suggested in [10] for the derivation of the order conditions for ARKN methods. The coefficients of Scheifele's G-function method are dependent on the frequency ω and stepsize h. By using the ϕ-functions, the coefficients are dependent on only one variable $\nu = \omega\, h$.

The solution of (1.2) can be expressed as

$$y(x_n+h)=y(x_n)\ \cos(\nu)+hy'(x_n)\frac{\sin(\nu)}{\nu}+\frac{1}{\omega}\int_{x_n}^{x_{n+1}} g(x,y(x))\sin(\omega\,(x_{n+1}-x))\mathrm{d}x. \tag{3.14}$$

We carry out the change of variable $x=x_n+h\,z$ in (3.14) and we denote $\varphi(x)=g(x,y(x))$. Now the exact solution becomes

$$y(x_n+h)=y(x_n)\ \cos(\nu)+hy'(x_n)\frac{\sin(\nu)}{\nu}+h^2\int_0^1 \varphi(x_n+h\,z)\frac{\sin(\nu\,(1-z))}{\nu}\mathrm{d}z. \tag{3.15}$$

Suppose $\varphi(x)$ analytical, the Taylor series of $\varphi(x)$ is

$$\varphi(x_n+h\,z)=\sum_{j=0}^{\infty} h^j\,\varphi^{(j)}(x_n)\frac{z^j}{j!}. \tag{3.16}$$

We can write that

$$y(x_n+h)=y(x_n)\ \cos(\nu)+hy'(x_n)\frac{\sin(\nu)}{\nu}+\sum_{j=0}^{\infty} h^{j+2}\varphi^{(j)}(x_n)\int_0^1\frac{\sin(\nu\,(1-z))}{\nu}\frac{z^j}{j!}\mathrm{d}z. \tag{3.17}$$

Introducing the following notations

$$\phi_0(\nu)=\cos(\nu),\qquad \phi_1(\nu)=\frac{\sin(\nu)}{\nu},\qquad \phi_{j+2}(\nu)=\int_0^1\frac{\sin(\nu\,(1-z))}{\nu}\frac{z^j}{j!}\mathrm{d}z,\quad j\geq 0, \tag{3.18}$$

we arrive at the expression of the exact solution of the perturbed problem (1.2) in terms of ϕ-functions

$$y(x_n+h)=y_n\,\phi_0(\nu)+h\,y_n'\,\phi_1(\nu)+\sum_{j=0}^{\infty} h^{j+2}\,\varphi^{(j)}(x_n)\,\phi_{j+2}(\nu). \tag{3.19}$$

It is noted that the analytical solution of the harmonic oscillator is approximated exactly by the expansion (3.19).

Some interesting properties of the ϕ-functions are listed in the following theorem.

Theorem 1. 1. $\lim_{\nu\to 0}\phi_j(\nu)=\frac{1}{j!}, j\geq 0.$

2. *The ϕ-functions can be expressed as*

$$\phi_{2j}(\nu)=\frac{(-1)^j}{\nu^{2j}}\left(\cos(\nu)-\sum_{k=0}^{j-1}(-1)^k\frac{\nu^{2\,k}}{(2\,k)!}\right),\quad j\geq 0, \tag{3.20}$$

$$\phi_{2j+1}(\nu)=\frac{(-1)^j}{\nu^{2j+1}}\left(\sin(\nu)-\sum_{k=0}^{j-1}(-1)^k\frac{\nu^{2\,k+1}}{(2\,k+1)!}\right),\quad j\geq 0. \tag{3.21}$$

3. *The Taylor series expansions of the ϕ-functions are*

$$\phi_j(\nu)=\sum_{k=0}^{\infty}(-1)^k\frac{\nu^{2\,k}}{(2\,k+j)!},\quad j\geq 0. \tag{3.22}$$

4. $\phi_{j+1}(\nu)=\int_0^1\cos(\nu\,(1-z))\frac{z^j}{j!}\mathrm{d}z, j\geq 0.$
5. *We have the following recurrence relation*

$$\phi_j(\nu)+\nu^2\,\phi_{j+2}(\nu)=\frac{1}{j!},\quad j\geq 0. \tag{3.23}$$

The ϕ-functions are related to the Scheifele G-functions by $G_j(h)=h^j\,\phi_j(\nu), j\geq 0$. For further details and proofs about G-functions, see [23,6,21].

According to Theorem 1 (point 1) it is clear that when the frequency $\omega\to 0\,(\nu\to 0)$ the series (3.19) will become

$$y(x_n+h)=y(x_n)+h\,y'(x_n)+\sum_{j=0}^{\infty}\frac{h^{j+2}}{(j+2)!}y^{(j+2)}(x_n), \tag{3.24}$$

which is the classical Taylor expansion of the exact solution. Thus Scheifele's series (3.19) is a refinement of the classical Taylor method.

3.2. Formulation of the method

An s-stage TS method ((2.3) and (2.4)) can be rewritten in the following alternative form

$$k_i' = f\left(x_n + c_i\,h,\,(1+c_i)\,y_n - c_i\,y_{n-1} + h^2\sum_{j=1}^{s} a_{ij}\,k_j'\right),\quad i = 1,\ldots,s,$$

$$y_{n+1} = 2\,y_n - y_{n-1} + h^2\sum_{i=1}^{s} b_i(\nu)\,k_i'.$$

We can see that k_i' are evaluations of the function f at the points $x_n + c_i\,h$, where the second argument is an approximation to the solution at this point. Then, we have

$$y(x_n + c_i\,h) \approx (1+c_i)\,y_n - c_i\,y_{n-1} + h^2\sum_{j=1}^{s} a_{ij}\,k_j',\quad i = 1,\ldots,s.$$

For perturbed oscillators, i.e. when $f(x,y) = -\omega^2\,y + g(x,y)$, the internal stages Y_i are equal to

$$Y_i = (1+c_i)\,y_n - c_i\,y_{n-1} + h^2\sum_{j=1}^{s} a_{ij}\,(-\omega^2\,Y_j + k_j),$$

where

$$k_i = g(x_n + c_i\,h, Y_i),\quad i = 1,\ldots,s. \tag{3.25}$$

The coefficients a_{ij} represent the weights of the quadrature formulas used in the approximation of the internal stages.

The final stage is determined as follows. We can avoid the calculation of the first derivative of the solution of (3.15) by adding this expression with positive and negative stepsize to get

$$y(x_n + h) = 2\,\phi_0(\nu)\,y(x_n) - y(x_n - h) + h^2\int_{-1}^{1}\frac{\sin(\nu\,(1-|z|))}{\nu}\,\varphi(x_n + h\,z)\mathrm{d}z. \tag{3.26}$$

We shall approximate the exact solution by using the quadrature formula

$$\int_{-1}^{1}\frac{\sin(\nu\,(1-|z|))}{\nu}\,\varphi(x_n + h\,z)\mathrm{d}z \approx \sum_{i=1}^{s} b_i(\nu)\,k_i,$$

where the k-values are given by (3.25).

Altogether, we arrive at the following definition.

Definition 1. An s-stage Scheifele two-step (STS) method for the numerical integration of the IVP (1.2) is given by the scheme

$$Y_i = (1+c_i(\nu))\,y_n - c_i(\nu)\,y_{n-1} + h^2\sum_{j=1}^{s} a_{ij}(\nu)\left(-\omega^2\,Y_j + g(x_n + c_j(\nu)\,h, Y_j)\right),\quad 1,\ldots,s,$$

$$y_{n+1} = 2\,\phi_0(\nu)\,y_n - y_{n-1} + h^2\sum_{i=1}^{s} b_i(\nu)\,g(x_n + c_i(\nu)\,h, Y_i), \tag{3.27}$$

which can be expressed in Butcher notation by the table of coefficients

$$\begin{array}{c|ccc} c_1(\nu) & a_{11}(\nu) & \ldots & a_{1s}(\nu)\\ \vdots & \vdots & \ddots & \vdots\\ c_s(\nu) & a_{s1}(\nu) & \ldots & a_{ss}(\nu)\\ \hline & b_1(\nu) & \ldots & b_s(\nu)\end{array} = \begin{array}{c|c} c(\nu) & A(\nu)\\ \hline & b^{\mathrm{T}}(\nu)\end{array}.$$

From the next section, we remove the argument ν in the coefficients of the method. Remark that when $\omega \to 0$, STS methods reduce to classical TS methods.

As said, the convergence of a method is covered by consistency and zero-stability. The consistency (i.e. order is at least 1) follows from Section 4. The theorem in [18] says that any method applied to $y'' = 0$ with the resulting difference equation

$$y_{n+1} + a_1(\nu)\,y_n + y_{n-1} = 0,$$

is zero-stable if $a_1(\nu) = -2 + \mathcal{O}(\nu^q)$, $q > 2$. Using Theorem 1 (point 3) it is easy to see that STS methods are zero-stable.

4. Order conditions for STS methods

Our next aim is to derive order conditions for STS methods by adapting the recently developed B2-series theory in [4]. In what follows, the reader is referred to that paper for all the definitions and notations. The theory of B2-series is applicable only to one-step methods. So we have to search for a one-step formulation of STS methods. A modification of Coleman's proofs at several places will deliver the requested order conditions.

4.1. Adapted B2-series

Repeated differentiation of φ with respect to the independent variable x gives

$$\begin{aligned}
&\varphi^{(0)} = g(y),\\
&\varphi^{(1)} = g^{(1)}(y)(y'),\\
&\varphi^{(2)} = g^{(2)}(y)(y', y') + g^{(1)}(y)(f(y)),\\
&\varphi^{(3)} = g^{(3)}(y)(y', y', y') + 3\,g^{(2)}(y)(y', f(y)) + g^{(1)}(y)(f^{(1)}(y)(y')),\\
&\dots
\end{aligned}$$

The difference with the classical theory lies in the fact that every elementary differential starts with a Fréchet-derivative of g instead of f. The following definition explains how each elementary differential can be associated with a rooted tree.

Definition 2. The function G on $T_2 \setminus \{\emptyset, \tau'\}$ is defined by

1. $G(\tau)(y, y') = g$.
2. If $t = [t_1, \dots, t_m]_2 \in T_2$, then
$$G(t)(y, y') = g^{(m)}(y)\left(F(t_1)(y, y'), \dots, F(t_m)(y, y')\right),$$
where the function F is recursively defined in Definition 3 of [4].

Analogously to the classical theory, it is obvious that

$$\varphi^{(j)} = \sum_{\substack{t\in T_2\\ \rho(t)=j+2}} \alpha(t)\, G(t)(y, y'), \tag{4.28}$$

where $\alpha(t)$ represents the number of distinct monotonic labellings of the vertices of $t \in T_2$.

B2-series are defined in Definition 4 of [4]. Here that definition is adopted more pertinently for our methods.

Definition 3. Let β be a mapping from T_2 to $\mathbb{R}$. The adapted B2-series with coefficient function β is a formal series of the form

$$\tilde{B}(\beta, y) = \sum_{t\in T_2\setminus\{\emptyset,\tau'\}} \frac{h^{\rho(t)}}{\rho(t)!}\alpha(t)\,\beta(t)\,G(t)(y, y').$$

Coleman's fundamental lemma is then reformulated for the adapted case as follows.

Lemma 1. *Let $B(\beta, y)$ be a classical B2-series. Then $h^2\, g(B(\beta, y))$ is an adapted B 2-series,*

$$h^2\, g(B(\beta, y)) = \tilde{B}(\beta'', y),$$

with

$$\beta''(\emptyset) = \beta''(\tau') = 0, \quad \beta''(\tau) = 2,$$

and for all other $t = [t_1, \dots, t_m]_2 \in T_2$,

$$\beta''(t) = \rho(t)\,(\rho(t) - 1)\prod_{i=1}^{m} \beta(t_i).$$

The proof is essentially the same as the original proof.

4.2. One-step formulation

By defining $F_n := (y_{n+1} - \phi_0(\nu)\, y_n)/h$ the second equation of (3.27) can be expressed as a pair of equations

$$\begin{aligned}
&y_n = \phi_0(\nu)\, y_{n-1} + h\, F_{n-1},\\
&F_n = \phi_0(\nu)\, F_{n-1} - \omega\, \nu \phi_1^2(\nu) y_{n-1} + h\, (b^{\mathrm{T}} \otimes I)\, g(Y).
\end{aligned}$$

Now, the one-step formulation takes the form

$$u_n = M(\nu)\, u_{n-1} + h\Phi(u_{n-1}, h), \tag{4.29}$$

with

$$\begin{aligned} M(\nu) &= \begin{pmatrix} \phi_0(\nu) & 0 \\ -\omega\,\nu\,\phi_1^2(\nu) & \phi_0(\nu) \end{pmatrix}, \\ u_n &= \begin{pmatrix} y_n \\ F_n \end{pmatrix} \quad \text{and} \quad \Phi(u_{n-1}, h) = \begin{pmatrix} F_{n-1} \\ (b^{\mathrm{T}} \otimes I)\, g(Y) \end{pmatrix}, \end{aligned} \tag{4.30}$$

and Y is defined implicitly by

$$\begin{aligned} Y &= (e + c) \otimes y_n - c \otimes y_{n-1} + h^2\,(A \otimes I)\,(-\omega^2\, Y + g(Y)) \\ &= (\phi_0(\nu)\, e + (\phi_0(\nu) - 1)\, c) \otimes y_{n-1} + h\,(e + c) \otimes F_{n-1} + h^2\,(A \otimes I)\,(-\omega^2\, Y + g(Y)). \end{aligned} \tag{4.31}$$

4.3. Order conditions

The vector u_n is an approximation for $z(x_n, h)$, where

$$z(x, h) = \begin{pmatrix} y(x) \\ \dfrac{y(x + h) - \phi_0(\nu)\, y(x)}{h} \end{pmatrix}. \tag{4.32}$$

For exact starting values, the *lte* of the one-step formulation (4.29)–(4.31) is

$$d_n = z(x_n, h) - u_n.$$

This takes the form

$$d_n = z(x_n, h) - M(\nu)\, z(x_{n-1}, h) - h\,\Phi(x_{n-1}, h), \tag{4.33}$$

with

$$\Phi(x_{n-1}, h) = \begin{pmatrix} \dfrac{y(x_n) - \phi_0(\nu)\, y(x_{n-1})}{h} \\ (b^{\mathrm{T}} \otimes I)\, g(Y) \end{pmatrix}, \tag{4.34}$$

where Y is now defined implicitly by

$$Y = e \otimes\, y(x_{n-1}) + (e + c) \otimes (y(x_n) - y(x_{n-1})) + h^2\,(A \otimes I)\,(-\omega^2\, Y + g(Y)).$$

Following Theorem II.3.6 in [16] we have that:

Lemma 2. *The STS method (3.27) is of order p when $d_n = \mathcal{O}(h^{p+1})$.*

We are now ready to present one of the main results of this paper.

Theorem 2. *The sufficient conditions for a STS method (3.27) to be of order p are given by*

$$b^{\mathrm{T}}\,\Psi''(t) = \left(1 + (-1)^{\rho(t)}\right)\, \rho(t)!\,\phi_{\rho(t)}(\nu),$$

for trees $t \in T_2$ with $\rho(t) \le p + 1$. Recall that $\Psi''(t)$ is defined in [4].

Proof. Observing (4.32)–(4.34) we have that the first component of d_n is zero. Each component of the vector Y can be expanded as a B2-series

$$Y_i(x_n) = B(\psi_i, y(x_n)) = \sum_{t \in T_2} \frac{h^{\rho(t)}}{\rho(t)!}\, \alpha(t)\, \psi_i(t)\, F(t)(y_n, y_n'). \tag{4.35}$$

The coefficients $\psi_i(t)$ can be generated recursively by formulas (3.6)–(3.7) of [4]. We substitute the B2-series (4.35) into the second component of d_n and we apply Lemma 1. An easy calculation gives

$$\begin{aligned} &\frac{1}{h}\left(y(x_n + h) - 2\,\phi_0(\nu)\, y(x_n) + y(x_n - h) - h^2 \sum_{i=1}^{s} b_i\, g(Y_i(x_n))\right) \\ &= \frac{1}{h}\left(2 \sum_{j=1}^{\infty} h^{2j} \varphi_n^{(2j-2)} \phi_{2j}(\nu) - \sum_{i=1}^{s} b_i\, \tilde{B}\left(\psi_i'', y(x_n)\right)\right). \end{aligned} \tag{4.36}$$

Table 1
Sufficient order conditions

Tree t	$\rho(t)$	Order condition
t_{21}	2	$\sum_i b_i = 2\,\phi_2(\nu)$
t_{31}	3	$\sum_i b_i\, c_i = 0$
t_{41}	4	$\sum_i b_i\, c_i^2 = 4\,\phi_4(\nu)$
t_{42}		$\sum_{i,j} b_i\, a_{ij} = 2\,\phi_4(\nu)$
t_{51}	5	$\sum_i b_i\, c_i^3 = 0$
t_{52}		$\sum_{i,j} b_i\, c_i\, a_{ij} = 2\,\phi_4(\nu)$
t_{53}		$\sum_{i,j} b_i\, a_{ij}\, c_j = 0$
t_{61}	6	$\sum_i b_i\, c_i^4 = 48\,\phi_6(\nu)$
t_{62}		$\sum_{i,j} b_i\, c_i^2\, a_{ij} = 24\,\phi_6(\nu)$
t_{63}		$\sum_{i,j} b_i\, c_i\, a_{ij}\, c_j = -\frac{2}{3}\,\phi_4(\nu) + 8\,\phi_6(\nu)$
t_{64}		$\sum_{i,j,k} b_i\, a_{ij}\, a_{ik} = \phi_4(\nu) + 12\,\phi_6(\nu)$
t_{65}		$\sum_{i,j} b_i\, a_{ij}\, c_j^2 = 4\,\phi_6(\nu)$
t_{66}		$\sum_{i,j,k} b_i\, a_{ij}\, a_{jk} = 2\,\phi_6(\nu)$
t_{71}	7	$\sum_i b_i\, c_i^5 = 0$
t_{72}		$\sum_{i,j} b_i\, c_i^3\, a_{ij} = 24\,\phi_6(\nu)$
t_{73}		$\sum_{i,j} b_i\, c_i^2\, a_{ij}\, c_j = 0$
t_{74}		$\sum_{i,j,k} b_i\, c_i\, a_{ij}\, a_{ik} = 24\,\phi_6(\nu)$
t_{75}		$\sum_{i,j,k} b_i\, c_i\, a_{ij}\, a_{jk} = -\frac{1}{6}\,\phi_4(\nu) + 4\,\phi_6(\nu)$
t_{76}		$\sum_{i,j} b_i\, c_i\, a_{ij}\, c_j^2 = \frac{1}{3}\,\phi_4(\nu)$
t_{77}		$\sum_{i,j,k} b_i\, a_{ij}\, a_{ik}\, c_k = -\frac{1}{3}\,\phi_4(\nu) + 4\,\phi_6(\nu)$
t_{78}		$\sum_{i,j} b_i\, a_{ij}\, c_j^3 = 0$
t_{79}		$\sum_{i,j,k} b_i\, a_{ij}\, c_j\, a_{jk} = 2\,\phi_6(\nu)$
$t_{7,10}$		$\sum_{i,j,k} b_i\, a_{ij}\, a_{jk}\, c_k = 0$

With (4.28) in mind, the left term of (4.36) becomes

$$2\sum_{j=1}^{\infty} h^{2j}\varphi_n^{(2j-2)}\phi_{2j}(\nu) = \sum_{t\in T_2\setminus\{\emptyset,\tau'\}} \left(1+(-1)^{\rho(t)}\right) h^{\rho(t)}\,\alpha(t)\,\phi_{\rho(t)}(\nu)\,G(t)(y_n,y_n'). \tag{4.37}$$

The right side of (4.36) may be written as

$$\sum_{i=1}^{s} b_i\,\tilde{B}(\psi_i'',y_n) = \sum_{t\in T_2\setminus\{\emptyset,\tau'\}} \frac{h^{\rho(t)}}{\rho(t)!}\,\alpha(t)\,b_i\,\psi_i''(t)\,G(t)(y_n,y_n'). \tag{4.38}$$

The theorem follows when comparing (4.37) and (4.38). □

Sufficient order conditions up to order six are listed in Table 1. Taking into account that the coefficients of a STS method are ν-dependent it follows that:

Theorem 3. *The necessary and sufficient conditions for a STS method (3.27) to be of order p are given by*

$$b^{\mathrm{T}}\,\Psi''(t) = \left(1+(-1)^{\rho(t)}\right)\,\rho(t)!\,\phi_{\rho(t)}(\nu) + \mathcal{O}(h^{p+2-\rho(t)}),$$

for trees $t\in T_2$ with $\rho(t)\le p+1$.

Remark 1. When using the necessary and sufficient order conditions of Theorem 3 we have to consider the Taylor expansions of the ϕ-functions. The resulting coefficients are then simply polynomials in ν which reduce the computational cost when using variable stepsizes, see also [10]. To our knowledge, stepsize control for TS methods has not been investigated so far. Furthermore, in [10] we observe that the ARKN methods based on the necessary and sufficient order conditions are less accurate than methods based on the sufficient order conditions when using fixed stepsizes. Thus from now on, we consider only STS methods based on the sufficient order conditions of Theorem 2, see also Table 1.

Remark 2. Reconsidering Section 5 in [4] it is obvious that, in order to reduce the number of order conditions, the simplifying conditions for STS methods are the same as those for classical TS methods.

4.4. Error analysis

From the proof of Theorem 2 it follows that the *plte* of a pth-order STS method is given by

$$plte^{STS} = \frac{h^{p+2}}{(p+2)!}\sum_{\substack{t\in T_2\\ \rho(t)=p+2}} \alpha(t)\,\left(1+(-1)^{p+2} - b^{(0)^{\mathrm{T}}}\,\Psi''^{(0)}(t)\right)G(t)(y_n,y_n'),$$

where $b^{(0)^{\mathrm{T}}}$ and $\Psi''^{(0)}$ represents the b^{T}- and Ψ''-values of the corresponding classical TS method. The *plte* of this classical method for (1.1) reads

$$plte^{TS} = \frac{h^{p+2}}{(p+2)!} \sum_{\substack{t\in T_2 \\ \rho(t)=p+2}} \alpha(t) \left(1 + (-1)^{p+2} - b^{(0)^{\mathrm{T}}} \Psi''^{(0)}(t)\right) F(t)(y_n, y'_n). \tag{4.39}$$

In order to obtain a connection between $plte^{TS}$ and $plte^{STS}$ we need a relationship between $F(t)$ and $G(t)$. This can be easily seen as follows. We consider trees in which the root starts with a chain of 3 vertices (including the root) having exactly one son. We call such a tree a *semi-tall tree*. We denote by T_2^* the set of semi-tall trees. The *truncated tree* t^- of a semi-tall tree t is obtained by deleting the first two vertices. Clearly, the number of semi-tall trees of order $p+2$ is equal to the number of trees of order p. Using the above terminology, it is easy to see that

$$G(t)(y, y') = \begin{cases} F(t)(y, y') + \omega^2 F(t^-)(y, y') & \text{if } t \in T_2^*, \\ F(t)(y, y') & \text{if } t \notin T_2^*. \end{cases}$$

We conclude with

$$plte^{STS} = plte^{TS} + \omega^2 \frac{h^{p+2}}{(p+2)!} \sum_{\substack{t\in T_2^* \\ \rho(t)=p+2}} \alpha(t) \left(1 + (-1)^{p+2} - b^{(0)^{\mathrm{T}}} \Psi''^{(0)}(t)\right) F(t^-)(y_n, y'_n). \tag{4.40}$$

For the calculation of the error constant, E_{p+1}^{STS}, we have to consider the coefficients of $F(t)(y_n, y'_n)$ and the coefficients of $\omega^2 F(t^-)(y_n, y'_n)$ in (4.40). Observing (4.39) and (4.40) it is clear that

$$E_{p+1}^{STS} = \left(\sum_{\substack{t\in T_2 \\ \rho(t)=p+2}} l_i \, (\mathrm{e}_{p+1}^{TS})^2(t_i) \right)^{1/2} \qquad \text{with } l_i = \begin{cases} 2 & \text{if } t \in T_2^*, \\ 1 & \text{if } t \notin T_2^*. \end{cases} \tag{4.41}$$

5. Linear stability analysis

Linear stability and phase-lag analysis of STS methods is also based on the model equation (2.7). However, this equation has to be rewritten in the following appropriate form

$$y'' = -\omega^2 y - \epsilon\, y, \quad \omega^2 + \epsilon > 0, \tag{5.42}$$

where ω represents an estimation of the dominant frequency λ of (2.7), and $\epsilon = \lambda^2 - \omega^2$ is the error of that estimation. This modified test equation is prompted by the work in [12] for ARKN methods. At first sight, one should believe that the estimated frequency ω should be equal to dominant frequency λ. This is generally a satisfying approach but in practical applications it is possible to obtain more accurate results for distinct values of λ and ω. The cubic oscillator

$$y'' = -y + \epsilon\, y^3, \qquad y(0) = 1, \qquad y'(0) = 1,$$

provides such an example. Although this is a nonlinear problem, for small ϵ-values we may apply linear stability analysis, resulting in $\lambda = 1$. However, Vigo-Aguiar et al. [33] have proved that more accurate results are obtained when selecting $\omega = \sqrt{1 - 0.75\,\epsilon}$.

A STS method (3.27) applied to (5.42) yields

$$\begin{aligned} Y &= (e + c)\, y_n - c\, y_n - (\nu^2 + z)\, A\, Y, \\ y_{n+1} &= 2\,\phi_0(\nu)\, y_n - y_{n-1} - z\, b^{\mathrm{T}}\, Y, \qquad \nu = \omega\, h, \qquad z = \epsilon\, h^2. \end{aligned}$$

Elimination of the vector Y gives the recurrence relation

$$y_{n+1} - S(\nu^2, z)\, y_n + P(\nu^2, z)\, y_{n-1} = 0, \tag{5.43}$$

where

$$S(\nu^2, z) = 2\,\phi_0(\nu) - z\, b^{\mathrm{T}} N^{-1} (e + c), \qquad P(\nu^2, z) = 1 - z\, b^{\mathrm{T}} N^{-1} c, \tag{5.44}$$

and

$$N = I + (\nu^2 + z)\, A, \qquad e = (1, \ldots, 1)^{\mathrm{T}}. \tag{5.45}$$

The characteristic equation is

$$\xi^2 - S(\nu^2, z)\, \xi + P(\nu^2, z) = 0. \tag{5.46}$$

Firstly, let us consider dissipative STS methods. Working with (5.46), we can ask, for a given method (i.e., a given ω), and a given test frequency λ, what restriction must be placed on the stepsize h to ensure that the stability condition

$$P(\nu^2, z) < 1 \quad \text{and} \quad |S(\nu^2, z)| < P(\nu^2, z) + 1, \tag{5.47}$$

is satisfied. This question can be answered by examining $S(\nu^2, z)$ and $P(\nu^2, z)$ in the ν–z plane. For ARKN methods such a stability analysis was introduced in [12]. The following definition was originally formulated in [5] for exponentially-fitted methods for (1.1). Here, it is adjusted in terms of the methods of concern.

Definition 4. For a dissipative STS method with $S(\nu^2, z)$ and $P(\nu^2, z)$ where $\nu = \omega h$ and $z = \epsilon h$, and ω and ϵ are given, the primary interval of absolute stability is the largest interval $(0, h_0)$ such that (5.47) holds for all stepsizes $h \in (0, h_0)$. If, when h_0 is finite, (5.47) holds also for $\gamma < h < \delta$, where $\gamma > h_0$ then the interval (γ, δ) is a secondary interval of absolute stability. The region of absolute stability is a region in the ν–z plane ($\nu > 0$), throughout which (5.47) holds. Any closed curve defined by

$$P(\nu^2, z) = 1 \quad \text{or} \quad |S(\nu^2, z)| = P(\nu^2, z) + 1,$$

is a stability boundary.

Likewise, for zero-dissipative STS methods the definitions of the *primary interval of periodicity* and the *region of periodicity* are evident.

In the particular case when the main frequency is exactly known (i.e. $z = 0$) we have for both dissipative and zero-dissipative methods that

$$S(\nu^2, 0) = 2\cos(\nu) \quad \text{and} \quad P(\nu^2, 0) = 1.$$

It follows that the ν-axis is a stability boundary. On this line the periodicity condition (2.12) is satisfied except when $\nu = n\pi$ for positive integer n.

In the dissipative case, when the frequency is not exactly known the stepsize has to be selected carefully. Here we show some sensible points.

Theorem 4. *For dissipative STS methods there exist values for ω and ϵ for which the primary interval of absolute stability is empty, except possibly for a discrete set of exceptional values of h determined by the chosen of ω.*

Proof. Consider the function F defined as

$$F(H^2) = b^{\mathrm{T}} (I + H^2 A)^{-1} c.$$

F is continuous and non-zero at $H^2 = \nu^2$, except possibly for a discrete set of ν-values. Excluding these exceptional ν-values we can find an interval $(-z_0, z_0)$ such that $F(\nu^2 + z)$ has the same sign for all $z \in (-z_0, z_0)$. It turns out that for such z-values the function P, as given in (5.44) and (5.45), has a different sign at the points $(\nu, -z)$ and (ν, z). From the absolute stability condition (5.47) it follows that a STS method which is stable at $(\nu, -z)$, is not stable at (ν, z). Thus we have proved the existence of empty primary intervals of absolute stability except for values $h = \nu/\omega$ where F is discontinuous or zero at $H^2 = \nu^2$. This concludes the proof. □

6. Phase-lag and dissipation analysis

For any method corresponding to the characteristic equation (5.46), the quantities

$$\phi(\nu^2, z) = H - \arccos\left(\frac{S(\nu^2, z)}{2\sqrt{P(\nu^2, z)}}\right), \qquad d(\nu^2, z) = 1 - \sqrt{P(\nu^2, z)}, \tag{6.48}$$

are called the phase-lag and the amplification error, respectively. As pointed out in [12] for ARKN methods, the analysis of the phase-lag and the dissipation becomes more useful if we introduce

$$\nu = \frac{\omega}{\sqrt{\omega^2 + \epsilon}} H, \qquad z = \frac{\epsilon}{\omega^2 + \epsilon} H^2, \tag{6.49}$$

in (6.48). So we arrive at the following definition.

Definition 5. The phase-lag order is q if

$$\phi(\nu^2, z) = c_\phi(\omega^2, \epsilon) H^{q+1} + \mathcal{O}(H^{q+3}), \tag{6.50}$$

and the dissipation order is r if

$$d(\nu^2, z) = c_d(\omega^2, \epsilon) H^{r+1} + \mathcal{O}(H^{r+3}). \tag{6.51}$$

$c_\phi(\omega^2, \epsilon)$ and $c_d(\omega^2, \epsilon)$ are called the phase-lag and dissipation functions, respectively.

In the particular case when the main frequency is exactly known (i.e. $z = 0$) the test equation (5.42) is integrated exactly and so there is no phase-error and no dissipation.

We investigate the phase properties when the main frequency is not exactly known. Let us define $C_j := b^{\mathrm{T}} A^{j-1} c$ and $U_j := b^{\mathrm{T}} A^{j-1} e$. Some algebraic manipulation gives

- STS method of order $p = 2k$:

$$S(\nu^2, z) = 2\sum_{j=0}^{k} \frac{(-1)^j}{(2j)!} H^{2j} + 2\sum_{j=k+1}^{\infty} \frac{(-1)^j}{(2j)!} H^{2j} \left(\frac{\omega^2}{\omega^2+\epsilon}\right)^{j-k} + \frac{\epsilon}{\omega^2+\epsilon} \sum_{j=k+1}^{\infty} (-1)^j (U_j + C_j) H^{2j}, \tag{6.52}$$

$$P(\nu^2, z) = 1 + \frac{\epsilon}{\omega^2+\epsilon} \sum_{j=k+1}^{\infty} (-1)^j C_j H^{2j}.$$

- STS method of order $p = 2k - 1$:

$$\begin{aligned} S(\nu^2, z) &= 2\sum_{j=0}^{k} \frac{(-1)^j}{(2j)!} H^{2j} + 2\sum_{j=k+1}^{\infty} \frac{(-1)^j}{(2j)!} H^{2j} \left(\frac{\omega^2}{\omega^2+\epsilon}\right)^{j-k} \\ &\quad + \frac{\epsilon}{\omega^2+\epsilon} (-1)^k C_k H^{p+1} + \frac{\epsilon}{\omega^2+\epsilon} \sum_{j=k+1}^{\infty} (-1)^j (U_j + C_j) H^{2j}, \end{aligned}$$

$$P(\nu^2, z) = 1 + \frac{\epsilon}{\omega^2+\epsilon} \sum_{j=k}^{\infty} (-1)^j C_j H^{2j}. \tag{6.53}$$

When substituting (6.52) and (6.53) in (6.48) and then considering the Taylor expansion with respect to H it is sufficient to retain the term with the lowest power. After tedious but straightforward calculations we have concluded with:

Theorem 5. 1. *Assume that the order p of a dissipative TS method is even (odd) and that the phase-lag order is $q = p (q = p+1)$. Then the corresponding STS method has also phase-lag order q. The leading term of the phase-lag (6.50) is*

$$c_\phi(\omega, \epsilon) = \frac{\epsilon}{\omega^2+\epsilon} c_\phi, \tag{6.54}$$

where c_ϕ is the phase-lag constant of the classical TS method.

2. *A dissipative TS method and the corresponding STS method have both the same dissipation order. The leading term of the dissipation (6.51) is*

$$c_d(\omega, \epsilon) = \frac{\epsilon}{\omega^2+\epsilon} c_d, \tag{6.55}$$

where c_d is the dissipation constant of the classical TS method.

From (6.54) it follows that the conditions for a STS method to have phase-lag order $q = p + 2$ (p: even) or $q = p + 3$ (p: odd) are exactly the same as those of the corresponding classical method. This establishes:

Corollary 6. *Assume that the order p of a TS method is even (odd) and that the phase-lag order is $q = p + 2$ ($q = p + 3$). Then the corresponding STS method has also phase-lag order q.*

In general, Scheifele's adaptation does not conserve the phase-lag order for dissipative TS methods. In contrast, we will show that the phase-lag order is always conserved in the zero-dissipative case. Taking into account the order conditions obtained in Section 4 and proceeding as in Section 9 of [4] we can reformulate Coleman's Theorem 6 for zero-dissipative STS methods as follows.

Theorem 7. *For the determination of the phase-lag order of a zero-dissipative STS method (3.27) we have to compute the scalar quantities $C_k = b^{\mathrm{T}} A^{k-1} c$ and $U_k = b^{\mathrm{T}} A^{k-1} e$ for $k = 1, 2, \ldots$. The phase-lag order is q iff $U_k = 2\phi_{2k}(\nu)$ for $k = 1, \ldots, [\frac{p+1}{2}]$ and $C_k = 0$ for $k = 1, \ldots, [\frac{p}{2}]$ but one of those conditions is not satisfied when p is replaced by $p + 1$.*

Corollary 8. *A zero-dissipative STS method and its corresponding classical method have both the same phase-lag order.*

The phase-lag function is also of the form (6.54).

Obviously we have in all cases that $c_\phi(\omega, 0) = c_d(\omega, 0) = 0$, $c_\phi(0, \epsilon) = c_\phi$ and $c_d(0, \epsilon) = c_d$. When an acceptable estimate of the dominant frequency is available (i.e. $\epsilon \approx 0$) the magnitude of the phase-lag (6.54) and the amplification error (6.55) are then much smaller than those of the corresponding classical method. Furthermore, the more accurate the estimate of the dominant frequency, the smaller the phase-lag and the amplification error.

7. Construction of explicit STS methods

In this section we study the construction of explicit STS methods with orders four and five. Both dissipative and zero-dissipative methods are presented. The construction procedure in the classical case was previously considered in [13].

7.1. Methods using two function evaluations per step

Consider the explicit STS method defined by the table of coefficients

$$\begin{array}{c|ccc} -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ c_3 & a_{31} & a_{32} & 0 \\ \hline & b_1 & b_2 & b_3 \end{array}.$$

Under the simplifying assumptions (see [4])

$$A\,e = \frac{c^2+c}{2}, \tag{7.56}$$

the sufficient order conditions up to order four are

$$b^{\mathrm{T}} e = 2\,\phi_2(\nu), \qquad b^{\mathrm{T}} c = 0, \qquad b^{\mathrm{T}} c^2 = 4\,\phi_4(\nu), \qquad b^{\mathrm{T}} c^3 = 0, \qquad b^{\mathrm{T}} A\,c = 0. \tag{7.57}$$

We have the unique solution

$$b_1 = b_3 = 2\,\phi_4(\nu), \qquad b_2 = -4\,\phi_4(\nu) + 2\,\phi_2(\nu), \qquad c_3 = 1, \qquad a_{31} = 0, \qquad a_{32} = 1. \tag{7.58}$$

When $\nu \to 0$ the method reduces to the explicit Numerov method in [1]. Remark that the values (7.58) are obtained in a different way in [30]. A stability and phase-lag analysis is also included in that paper.

7.2. Methods using three function evaluations per step

Next, we analyze the construction of explicit STS methods defined by the table of coefficients

$$\begin{array}{c|cccc} -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ c_3 & a_{31} & a_{32} & 0 & 0 \\ c_4 & a_{41} & a_{42} & a_{43} & 0 \\ \hline & b_1 & b_2 & b_3 & b_4 \end{array}. \tag{7.59}$$

7.2.1. Dissipative fifth-order methods

The sufficient order conditions up to order five are given by (7.56) and (7.57) with, in addition

$$b^{\mathrm{T}} c^4 = 48\,\phi_6(\nu), \qquad b^{\mathrm{T}} (c\,.\,A\,c) = -\frac{2}{3}\,\phi_4(\nu) + 8\,\phi_6(\nu), \qquad b^{\mathrm{T}} A\,c^2 = 4\,\phi_6(\nu). \tag{7.60}$$

Solving Eqs. (7.56), (7.57) and (7.60), the coefficients (7.59) are determined in terms of the arbitrary parameter c_3. Two different strategies will be described in order to get an optimal method. A first option is to determine c_3 so that the error constant E_6^{STS} (4.41) is as small as possible. The second option is to choose c_3 so that the method has phase-lag order eight.

* *STS method with minimized error constant*

When minimizing the error constant E_6^{STS}, we obtain a value for c_3 which is very close (within a distance $<10^{-3}$) to those of a classical method in [13], $c_3 = 63/100$. For this reason we adopt Franco's method and we conclude with the coefficients

$$\begin{aligned}
&a_{31} = \frac{126\,651}{2000\,000}, \qquad a_{32} = \frac{900\,249}{2000\,000}, \qquad a_{41} = \frac{100\,S_1\,S_2\,(720\,000\,\phi_6^2 - 124\,158\,\phi_6\,\phi_4 + 6031\,\phi_4^2)}{305\,488\,243\,\phi_4^4}, \\
&a_{42} = \frac{S_1\,S_2\,(-8000\,000\,\phi_6^2 + 886\,200\,\phi_6\,\phi_4 + 2849\,\phi_4^2)}{13\,119\,127\,\phi_4^4}, \qquad a_{43} = \frac{20\,000\,S_1\,S_2\,S_3\,\phi_6}{2138\,417\,701\,\phi_4^4}, \\
&b_1 = \frac{6\,(40\,000\,\phi_6 - 1323\,\phi_4)\,\phi_4}{163\,S_1}, \\
&b_2 = \frac{2\,(15\,338\,\phi_4^2 - 240\,000\,\phi_6\,\phi_4 - 3969\,\phi_4\,\phi_2 + 75\,600\,\phi_2\,\phi_6)}{189\,S_2}, \\
&b_3 = \frac{400\,000\,000\,(12\,\phi_6 - \phi_4)\,\phi_4}{30\,807\,S_3}, \qquad b_4 = \frac{3748\,322\,\phi_4^4}{9\,S_1\,S_2\,S_3}, \qquad c_3 = \frac{63}{100}, \qquad c_4 = \frac{3\,S_2}{37\,\phi_4}, \\
&S_1 = 600\,\phi_6 - 13\,\phi_4, \qquad S_2 = 400\,\phi_6 - 21\,\phi_4, \qquad S_3 = 40\,000\,\phi_6 - 2877\,\phi_4.
\end{aligned} \tag{7.61}$$

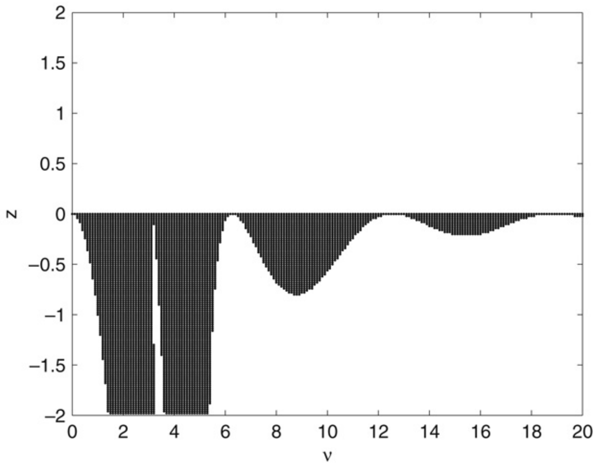

Fig. 1. Stability region of STS method (7.61).

The region of absolute stability is drawn in Fig. 1. The expressions for the phase-lag and dissipation associated to this method are given by

$$\phi(\nu, z) = \frac{23\,\epsilon}{378\,000\,(\omega^2+\epsilon)}\,H^7 + \mathcal{O}(H^9), \qquad d(\nu, z) = -\frac{37\,\epsilon}{216\,000(\omega^2+\epsilon)}\,H^6 + \mathcal{O}(H^8).$$

It should be reminded that we have used the substitution (6.49) in the above expressions (since there are no ν and z, but ω^2, ϵ and H^2).

* *STS Method with phase-lag order eight*

Following Corollary 6 the condition that imposes phase-lag order eight is the same as that for the classical method. In the classical case, phase-lag order eight is achieved when $c_3 = 25/28$, see [13]. Guided by Franco's method, we conclude with the coefficients

$$\begin{aligned}
&a_{31} = \frac{1325}{43\,904}, \qquad a_{32} = \frac{35\,775}{43\,904}, \qquad a_{41} = \frac{28\,S_1\,S_2\,(18\,816\,\phi_6^2 - 2186\,\phi_6\,\phi_4 + 53\,\phi_4^2)}{4293\,\phi_4^4},\\
&a_{42} = -\frac{S_1\,S_2\,(526\,848\,\phi_6^2 - 51\,800\,\phi_6\,\phi_4 + 475\,\phi_4^2)}{2025\,\phi_4^4}, \qquad a_{43} = \frac{1568\,S_1\,S_2\,S_3\,\phi_6}{107\,325\,\phi_4^4},\\
&b_1 = \frac{2\,(9408\,\phi_6 - 625\,\phi_4)\,\phi_4}{53\,S_2},\\
&b_2 = \frac{2\,(1418\,\phi_4^2 - 625\,\phi_4\,\phi_2 - 18\,816\,\phi_6\,\phi_4 + 8400\,\phi_2\,\phi_6)}{25\,S_1},\\
&b_3 = \frac{2458\,624\,(12\,\phi_6 - \phi_4)\,\phi_4}{1325\,S_3}, \qquad b_4 = \frac{162\,\phi_4^4}{S_1\,S_2\,S_3}, \qquad c_3 = \frac{25}{28}, \qquad c_4 = \frac{S_1}{3\,\phi_4},\\
&S_1 = 336\,\phi_6 - 25\,\phi_4, \qquad S_2 = 168\,\phi_6 - 11\,\phi_4, \qquad S_3 = 9408\,\phi_6 - 775\,\phi_4.
\end{aligned} \tag{7.62}$$

The region of absolute stability is drawn in Fig. 2. The phase-lag and dissipation for this method are

$$\phi(\nu, z) = -\frac{(199\,\omega^2 + 182\,\epsilon)\,\epsilon}{101\,606\,400\,(\omega^2+\epsilon)^2}\,H^9 + \mathcal{O}(H^{11}), \qquad d(\nu, z) = -\frac{\epsilon}{20\,160(\omega^2+\epsilon)}\,H^6 + \mathcal{O}(H^8).$$

7.2.2. *Zero-dissipative fourth-order method with phase-lag order six*

Here we investigate how we can obtain zero-dissipative methods. Following Theorem 7 the method has phase-lag order six when

$$b^{\mathrm{T}} A^2\, c = 0, \qquad b^{\mathrm{T}} A^2\, e = 2\,\phi_6(\nu). \tag{7.63}$$

We find $c_3 = 1$ which is incompatible with the fifth-order conditions (7.60), and the order of the method should be restricted to four. Solving Eqs. (7.56), (7.57) and (7.63) we obtain the coefficients in terms of arbitrary parameters c_3 and c_4. The error constant E_5^{STS} (4.41) should be as small as possible so that we have $c_4 = (5\,c_3 - 2)/(5\,c_3 - 5)$, just like in Franco's original case. It is easy to verify that the method reaches order five for linear systems of ODEs

$$y'' = -\omega^2\, y + g(x). \tag{7.64}$$

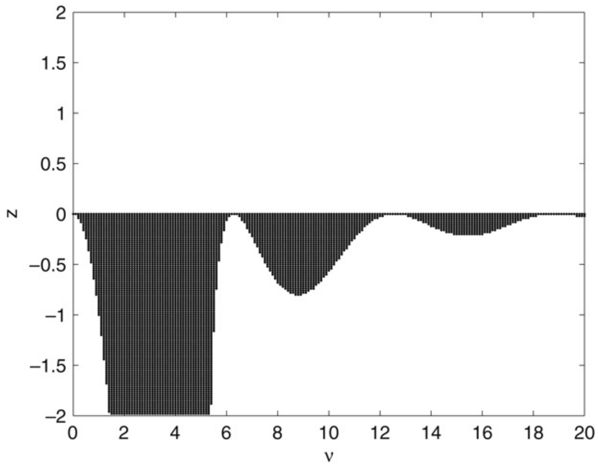

Fig. 2. Stability region of STS method (7.62).

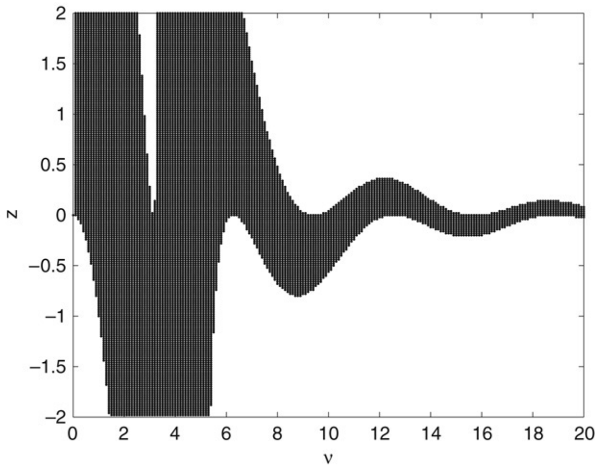

Fig. 3. Periodicity region of STS method (7.65).

In the classical case the free parameter c_3 is chosen so that the resulting method is optimized for the class of linear problems (7.64). Here, in order to calculate the error constant when solving (7.64), we have to consider the coefficients of the seventh-order elementary differentials $f^{(5)}(x)(y', y', y', y', y'), f^{(1)}(y)\left(f^{(3)}(x)(y', y', y')\right)$ and $\omega^2 f^{(3)}(x)(y', y', y')$. The other seventh-order elementary differentials remain zero for (7.64). Minimizing this error constant we obtain $c_3 = 13/20$. For comparison, in the classical case Franco [13] obtained $c_3 = 33/50$. The following coefficients are found

$$\begin{aligned}
&a_{31} = 0, \quad a_{32} = \frac{429}{800}, \quad a_{41} = \frac{38\,200\,\phi_6}{79\,233\,\phi_4}, \quad a_{42} = -\frac{5\,(7640\,\phi_6 + 637\,\phi_4)}{31\,213\,\phi_4}, \\
&a_{43} = \frac{764\,000\,\phi_6}{1030\,029\,\phi_4}, \quad b_1 = -\frac{6\,\phi_4}{11}, \quad b_2 = -\frac{596\,\phi_4}{65} + 2\,\phi_2, \quad b_3 = \frac{128\,000\,\phi_4}{27\,313}, \\
&b_4 = \frac{4802\,\phi_4}{955}, \quad c_3 = \frac{13}{20}, \quad c_4 = -\frac{5}{7}.
\end{aligned} \tag{7.65}$$

The region of periodicity is drawn in Fig. 3, and the phase-lag is

$$\phi(\nu, z) = -\frac{\epsilon}{40320\,(\omega^2 + \epsilon)} H^7 + \mathcal{O}(H^9).$$

8. Numerical experiments

In order to evaluate the effectiveness of the new methods derived above we consider several model problems. The new method has been compared with other explicit TS codes proposed in the literature. The criterion used in the numerical

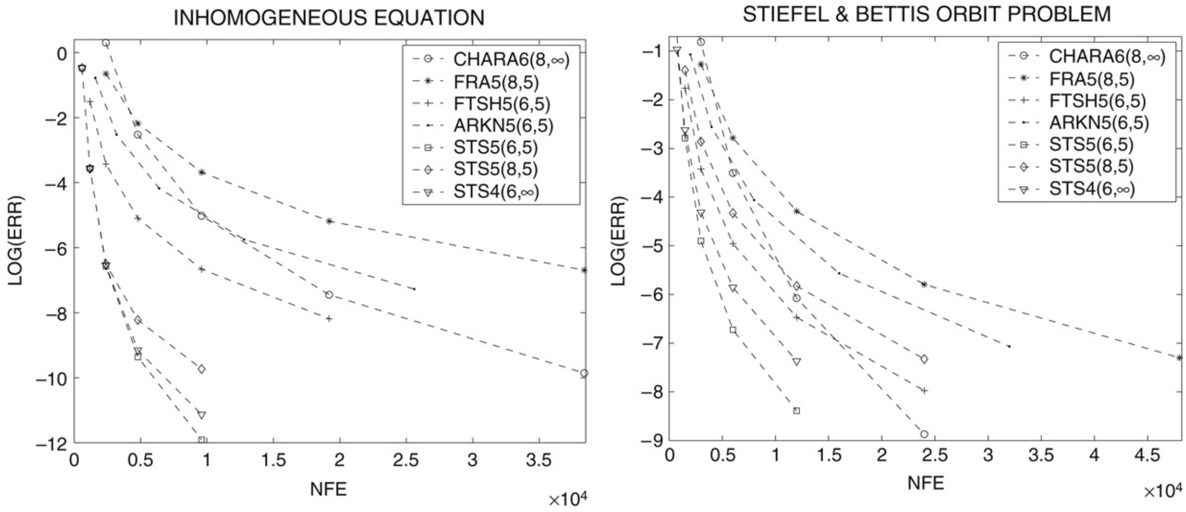

Fig. 4. Efficiency curves of the methods for Problems 1 and 2.

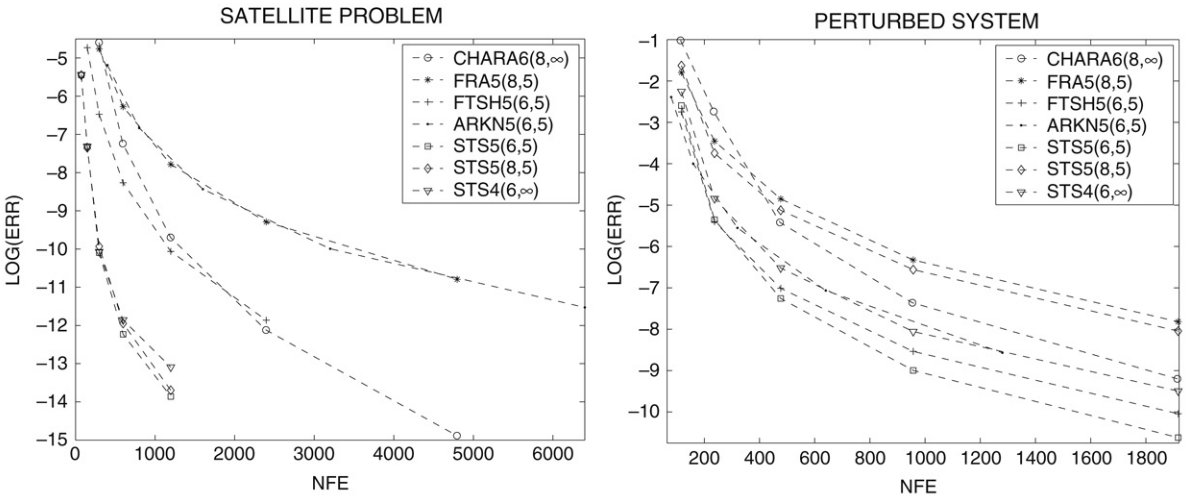

Fig. 5. Efficiency curves of the methods for Problems 3 and 4.

comparisons is the usual test based on computing the maximum global error over the whole integration interval. In Figs. 4 and 5 we have depicted the efficiency curves for the tested codes. These figures show the decimal logarithm of the maximum global error versus the computational error measured by the number of function evaluations required by each code. The algorithms used in the comparisons have been denoted by

- CHARA6(8, ∞): Zero-dissipative method derived in [2].
- FRA5(8, 5): Classical method derived in [13].
- FTSH5(6, 5): Phase-fitted and amplification-fitted method derived in [29].
- ARKN5(6, 5): Scheifele RKN method derived in [11].
- STS5(6, 5): STS method (7.61).
- STS5(8, 5): STS method (7.62).
- STS4(6, ∞): STS method (7.65).

Here, $A(B, C)$ means that the method has order A, phase-lag order B and dissipation order C.
We have used the following five model problems:

Problem 1. An inhomogeneous equation studied in [32]:

$$y'' = -100\,y + 99\sin(x), \qquad y(0) = 1, \qquad y'(0) = 11.$$

The exact solution is given by:

$$y(x) = \cos(10\,x) + \sin(10\,x) + \sin(x).$$

It consists of a rapidly and slowly oscillating function; the slowly varying function is due to the inhomogeneous term. The equation has been solved in the interval [0, 100] with fitted frequency $\omega = 10$. The numerical results stated in Fig. 4 have been computed with stepsizes $h = 2^{-j}$, $j = 2, \ldots, 6$ for CHARA6(8, ∞) and FTSH5(6, 5), $j = 3, \ldots, 7$ for FRA5(8, 5), $j = 1, \ldots, 5$ for STS5(6, 5), STS5(8, 5) and STS4(6, ∞), $j = -1, \ldots, 3$ for ARKN5(6, 5).

Problem 2. An "almost periodic" orbit problem studied in [27]:

$$z'' = -z + 0.001\mathrm{e}^{\mathrm{i}\,x}, \qquad z(0) = 1, \qquad z'(0) = 0.9995\,\mathrm{i}.$$

The equation has been solved in the interval [0, 1000] with fitted frequency $\omega = 1$. The exact solution is given by:

$$z(x) = (1 - 0.0005\mathrm{i}\,x)\mathrm{e}^{\mathrm{i}\,x}.$$

The solution represents a motion of a perturbation of a circular orbit in the complex plane. The problem may be solved either as a single equation in complex arithmetic or as a pair of uncoupled equations. The numerical results stated in Fig. 4 have been computed with stepsizes $h = 2^{-j}$, $j = -2, \ldots, 2$ for CHARA6(8, ∞), STS5(6, 5) and STS4(6, ∞), $j = -1, \ldots, 3$ for FTSH5(6, 5), ARKN5(6, 5) and STS5(8, 5), $j = 0, \ldots, 4$ for FRA5(8, 5).

Problem 3. A satellite problem was studied in [9].

We consider the problem of determining the position of an earth satellite. The equations of motion have been expressed in focal variables (see [8,9]). The coordinates of the basic set of focal variables are three components (y_1, y_2, y_3) of the direction vector of the particle and the inverse u of the radial distance. In this formulation the satellite problem can be formulated in four decoupled perturbed harmonic oscillators with unit frequency:

$$\begin{aligned} &y_i'' + y_i = Q_i, \quad i = 1, 2, 3, \\ &u'' + u = \frac{\mu}{c^2} + Q, \end{aligned} \tag{8.66}$$

where μ is the reduced mass, while Q_i and Q denote the corresponding perturbation terms. We consider the almost periodic equatorial orbit with the zonal harmonic coefficient J_2 taken as the perturbation parameter. We have neglected higher-order terms of J_2. The system of equations (8.66) can be written in the form

$$\begin{aligned} &y_i'' + y_i = 0, \quad i = 1, 2, 3, \\ &u'' + u = \frac{\mu}{c^2} + 12\frac{J_2}{c^2}u^2, \end{aligned} \tag{8.67}$$

where c is the angular momentum and it can be considered as a constant. The solutions of the first three oscillators are trivial. Thus we have focused on the last equation. We consider the domain of integration $[\pi, 100]$. The initial conditions are given by

$$u(\pi) = \frac{\mu\,(1-e)}{c^2}, \qquad u'(\pi) = 0.$$

For our numerical purpose we consider orbits with eccentricity $e = 0.99$. In this case:

$$\frac{\mu}{c^2} = \frac{100}{20\,895}, \qquad \frac{J_2}{c^2} = \frac{50}{20\,895\,000}.$$

The error has been calculated using a reference solution obtained by means of the perturbation techniques developed in [7]. The numerical results stated in Fig. 5 have been computed with stepsizes $h = (1 - \pi/100)\,2^{-j}$, $j = -1, \ldots, 3$ for CHARA6(8, ∞) and FTSH5(6, 5), $j = 0, \ldots, 4$ for FRA5(8, 5) and ARKN5(6, 5), $j = -2, \ldots, 2$ for STS5(6, 5), STS5(8, 5) and STS4(6, ∞).

Problem 4. A perturbed system was studied in [10].

As an example of a system we consider

$$\begin{aligned} &y_1'' = -25\,y_1 - \epsilon\,(y_1^2 + y_2^2) + \epsilon\,f_1(x), \qquad y_1(0) = 1, \qquad y_1'(0) = 0, \\ &y_2'' = -25\,y_2 - \epsilon\,(y_1^2 + y_2^2) + \epsilon\,f_2(x), \qquad y_2(0) = \epsilon, \qquad y_2'(0) = 5, \end{aligned}$$

where

$$\begin{aligned} &f_1(x) = 1 + \epsilon^2 + 2\,\epsilon\,\sin(5\,x + x^2) + 2\,\cos(x^2) + (25 - 4\,x^2)\sin(x^2), \\ &f_2(x) = 1 + \epsilon^2 + 2\,\epsilon\,\sin(5\,x + x^2) - 2\,\sin(x^2) + (25 - 4\,x^2)\,\cos(x^2). \end{aligned}$$

In our test we choose $\epsilon = 10^{-3}$. The system has been solved in the interval $[0, 5]$ with $\omega = 5$. The analytical solution is given by:

$$y_1(x) = \cos(5\,x) + \epsilon\,\sin(x^2), \qquad y_2(x) = \sin(5\,x) + \epsilon\,\cos(x^2).$$

The numerical results stated in Fig. 5 have been computed with stepsizes $h = 2^{-j}$, $j = 1, \ldots, 5$ for CHARA6(8, ∞), $j = 2, \ldots, 6$ for the other codes.

9. Conclusions

Scheifele's G-function methods are designed in such a way that the exact integration of the homogeneous solution of perturbed oscillators (1.2) is automatically included. The methods take care of the evaluation of the inhomogeneous part of (1.2), i.e. $g(x, y)$. We have applied Scheifele's approach to TS methods for an accurate and efficient integration of (1.2). The resulting methods, called STS methods, have coefficients dependent on $\nu = \omega\,h$, where ω is a specified angular frequency. Classical TS methods are the limiting forms of STS methods as $\omega \to 0$.

This paper provides a theoretical framework for the derivation of STS methods. One of our main aims is to develop the order conditions for this new type of methods. It is found that STS methods share some important properties with the corresponding classical TS methods such as zero-stability, the dissipation order and, under some conditions, with the phase-lag order. On the contrary, the stability properties are very different from the classical method and they depend on the fitted frequency and the stepsize. When the main frequency of the problem is exactly known stability problems will never occur, except for a discrete set of exceptional values of the stepsize. When the dominant frequency is not exactly known some care is required when selecting the stepsize.

In particular, we have demonstrated the validity of the theory with explicit fourth- and fifth-order STS methods. The new methods are adaptations of the classical TS methods in [13]. In most cases, the dissipative STS method (7.61) with minimized error constant outperforms all the other methods considered. In contrast with the results of the phase-fitted and amplification-fitted methods in [31], it turns out that the accuracy of STS methods is mostly determined by its usual local truncation error rather than by its phase-lag.

Our task is restricted to scalar equations or systems involving only one frequency. When solving systems with more than one frequency, or more general, systems of the form

$$y'' = K\,y + g(x, y), \tag{9.68}$$

the resulting methods have coefficients which are functions of the matrix $h^2\,K$. So their evaluation is not direct. To overcome this difficulty, together with some other troubles, Franco [14] has modified ARKN methods for oscillatory systems of the form (9.68). The extension of Franco's approach to the STS methods considered here might be an interesting suggestion for some future work.

References

[1] M.M. Chawla, Numerov made explicit has better stability, BIT 24 (1984) 117–118.
[2] M.M. Chawla, P.S. Rao, An explicit sixth-order method with phase-lag of order eight for $y'' = f(t, y)$, J. Comput. Appl. Math. 17 (1987) 365–368.
[3] J.P. Coleman, Numerical methods for $y'' = f(x, y)$ via rational approximations for the cosine, IMA J. Numer. Anal. 9 (1989) 145–165.
[4] J.P. Coleman, Order conditions for a class of two-step methods for $y'' = f(x, y)$, IMA J. Numer. Anal. 23 (2003) 197–220.
[5] J.P. Coleman, L.Gr. Ixaru, P-stability and exponential-fitting methods for $y'' = f(x, y)$, IMA J. Numer. Anal. 16 (1996) 179–199.
[6] V. Fairén, P. Martín, J.M. Ferrándiz, Numerical tracking of small deviations from analytically known periodic orbits, Comput. Phys. 8 (1994) 455–461.
[7] J.M. Farto, A.B. González, P. Martín, An algorithm for the systematic construction of solutions to perturbed problems, Comput. Phys. Commun. 111 (1998) 110–132.
[8] J.M. Ferrándiz, A general canonical transformation increasing the number of variables with applications to the two-body problem, Celest. Mech. 41 (1988) 343–357.
[9] J.M. Ferrándiz, M.E. Sansaturio, J.R. Pojman, Increased accuracy of computations in the main satellite problem through linearization methods, Celest. Mech. Dynam. Astronom. 53 (1992) 347–363.
[10] J.M. Franco, Runge–Kutta–Nyström methods adapted to the numerical integration of perturbed oscillators, Comput. Phys. Commun. 147 (2002) 770–787.
[11] J.M. Franco, A 5(3) pair of explicit ARKN methods for the numerical integration of perturbed oscillators, J. Comput. Appl. Math. 161 (2003) 283–293.
[12] J.M. Franco, Stability of explicit ARKN methods for perturbed oscillators, J. Comput. Appl. Math. 173 (2005) 389–396.
[13] J.M. Franco, A class of explicit two-step hybrid methods for second-order IVPs, J. Comput. Appl. Math. 187 (2006) 41–57.
[14] J.M. Franco, New methods for oscillatory systems based on ARKN methods, Appl. Numer. Math. 56 (2006) 1040–1053.
[15] A.B. González, P. Martín, J.M. Farto, A new family of Runge–Kutta type methods for the numerical integration of perturbed oscillators, Numer. Math. 82 (1999) 635–646.
[16] E. Hairer, S.P. Nørsett, G. Wanner, Solving Ordinary Differential Equations I, Nonstiff Problems, 2nd ed., in: Springer Series in Computational Mathematics, Berlin, 1993.
[17] P. Henrici, Discrete Variable Methods in Ordinary Differential Equations, Wiley, New York, 1962.
[18] L.Gr. Ixaru, M. Rizea, Numerov method maximally adapted to the Schrödinger equation, J. Comput. Phys. 73 (1987) 306–324.
[19] J.D. Lambert, I.A. Watson, Symmetric multistep methods for periodic initial-value problems, J. Inst. Math. Appl. 18 (1976) 189–202.
[20] D.J. López, P. Martín, J.M. Farto, Generalization of Störmer method for perturbed oscillators without explicit first dervatives, J. Comput. Appl. Math. 111 (1999) 123–132.
[21] P. Martín, J.M. Ferrándiz, Multistep numerical methods based on the Scheifele G-functions with application to satellite dynamics, SIAM J. Numer. Anal. 34 (1997) 359–375.
[22] L.R. Petzold, L.O. Jay, J. Yen, Numerical solution of highly oscillatory ordinary differential equations, Numerica Acta (1997) 437–483.
[23] G. Scheifele, On the numerical integration of perturbed linear oscillating systems, Z. Angew. Math. Phys. 22 (1971) 186–210.

[24] T.E. Simos, Explicit eight order methods for the numerical integration of initial-value problems with periodic or oscillating solutions, Comput. Phys. Commun. 119 (1999) 32–44.
[25] T.E. Simos, J. Vigo-Aguiar, On the construction of efficient methods for second order IVPS with oscillating solution, Internat. J. Modern Phys. C 12 (2001) 1453–1476.
[26] T.E. Simos, J. Vigo-Aguiar, Symmetric eighth algebraic order methods with minimal phase-lag for the numerical solution of the Schrodinger equation, J. Math. Chem. 31 (2002) 135–144.
[27] E. Stiefel, D.G. Bettis, Stabilization of Cowell's method, Numer. Math. 13 (1969) 154–175.
[28] Ch. Tsitouras, Explicit Numerov type methods with reduced number of stages, Comput. Math. Appl. 45 (2003) 37–42.
[29] H. Van de Vyver, A phase-fitted and amplification-fitted two-step hybrid method for second-order periodic initial value problems, Internat. J. Modern Phys. C 17 (2006) 663–675.
[30] H. Van de Vyver, An adapted explicit hybrid method of Numerov type for the numerical integration of perturbed oscillators, Appl. Math. Comput. 186 (2007) 1385–1394.
[31] H. Van de Vyver, Phase-fitted and amplification-fitted two-step hybrid methods for $y'' = f(x, y)$, J. Comput. Appl. Math. 209 (2007) 33–53.
[32] P.J. van der Houwen, B.P. Sommeijer, Explicit Runge–Kutta(–Nyström) methods with reduced phase errors for computing oscillating solutions, SIAM J. Numer. Anal. 24 (1987) 595–617.
[33] J. Vigo-Aguiar, T.E. Simos, J.M. Ferrándiz, Controlling the error growth in long-term numerical integration of perturbed oscillations in one or several frequencies, Proc. R. Soc. Lond. A 460 (2004) 561–567.